On Projection-Based Model Reduction for the Simulation of Nonlinear Systems

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Outline

Motivation

- System (typically discretization of (system of) PDE(s))

$$\mathbf{A}\mathbf{y} + \mathbf{F}(\mathbf{y};\theta) = \mathbf{B}\mathbf{u} + \mathbf{b}$$

  Parameter $\theta \in \Theta$, control $\mathbf{u} \in \mathcal{U}_{ad}$.
  (Both are parameters for purpose of model reduction.)

- (Deterministic) Optimal control

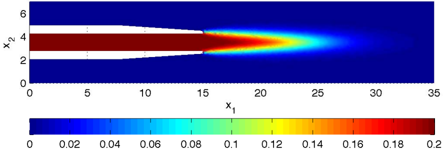
$$\begin{aligned} &\min\ J(\mathbf{y},\mathbf{u}) \\ &\text{s.t.}\ \ \mathbf{A}\mathbf{y} + \mathbf{F}(\mathbf{y};\theta_0) = \mathbf{B}\mathbf{u} + \mathbf{b}, \\ &\qquad \mathbf{u} \in \mathcal{U}_{ad}, \mathbf{y} \in \mathcal{Y}_{ad}. \end{aligned}$$

- Optimal control governed by PDEs with uncertain parameters (informal)

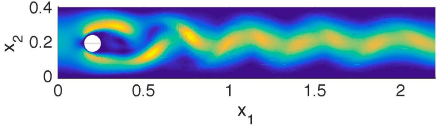
$$\begin{aligned} &\min\ \int_\Theta \rho(\theta) J(\mathbf{y}(\theta),\mathbf{u})\, d\theta \\ &\text{s.t.}\ \ \mathbf{A}\mathbf{y}(\theta) + \mathbf{F}(\mathbf{y}(\theta);\theta) = \mathbf{B}\mathbf{u} + \mathbf{b}, \quad \theta \in \Theta \\ &\qquad \mathbf{u} \in \mathcal{U}_{ad}, \\ &\qquad \mathbf{y}(\theta) \in \mathcal{Y}_{ad}, \quad \theta \in \Theta. \end{aligned}$$

Examples

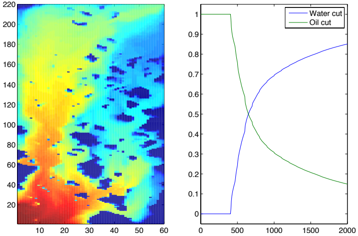
Nonlinear reaction advection diffusion



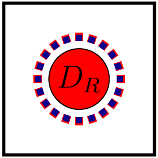
Flow control



Reservoir management



Direct field acoustic testing



Comp. domain, region of interest D_R, 20 speakers surrounding D_R.

In this talk

- Focus on simulation (solve $\mathbf{A}\mathbf{y} + \mathbf{F}(\mathbf{y}; \theta) = \mathbf{b}$).
- Detailed aspects of DEIM/EIM in finite element setting.
- Limits of DEIM/EIM.
- Error estimates.

Outline

Motivation

EIM and DEIM

EIM and DEIM for Finite Element Simulations

EIM and DEIM for Navier-Stokes

Error Estimate

Model Problem

Semilinear Advection-Diffusion-Reaction PDE

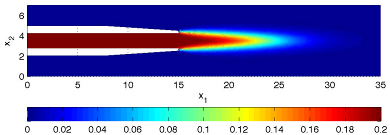
$$
\begin{aligned}
-\nu \Delta y + \beta \cdot \nabla y + f(y, \theta) &= 0, && \text{in } \Omega, \\
y &= h, && \text{on } \Gamma_D, \\
\nabla y \cdot n &= 0, && \text{on } \Gamma_N.
\end{aligned}
$$

Consider specific nonlinearity

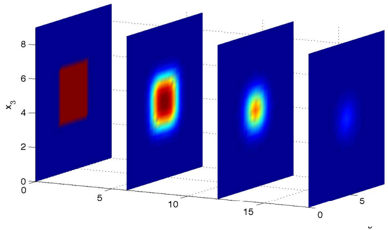
$$
f(y, \theta) = Ay(C - y)e^{-E/(D-y)}
$$

where C, D are known constants and $\theta = (\ln(A), E)$ are system parameters in $\Theta = [5.00, 7.25] \times [0.05, 0.15] \subset \mathbb{R}^2$.

2D



3D



- Semilinear Advection-Diffusion-Reaction PDE

$$\begin{aligned} -\nu\Delta y + \beta \cdot \nabla y + f(y,\theta) &= 0, && \text{in } \Omega, \\ y &= g, && \text{on } \Gamma_D, \\ \nabla y \cdot n &= 0, && \text{on } \Gamma_N. \end{aligned}$$

  Consider specific nonlinearity

$$f(y,\theta) = Ay(C-y)e^{-E/(D-y)}$$

  where C, D are known constants and $\theta = (\ln(A), E)$ are system parameters in $\Theta = [5.00, 7.25] \times [0.05, 0.15] \subset \mathbb{R}^2$.

- Weak form: Find $y \in H^1(\Omega)$ with $y = h$ on Γ_D such that

$$\int_\Omega \nu\nabla y \cdot \nabla v dx + \int_\Omega \beta \cdot \nabla y v dx + \int_\Omega f(y,\theta) v dx = 0$$

  for all $v \in H^1(\Omega)$ with $v = 0$ on Γ_D.

- Finite element discretization. Approximate

$$y_h(x) = \sum_{j=1}^{N} \mathbf{y}_j \phi_j(x) + \sum_{j=N+1}^{N+N_D} g(x_j)\phi_j(x)$$

where y_h satisfies

$$\int_\Omega \nu \nabla y_h \cdot \nabla \phi_i dx + \int_\Omega \beta \cdot \nabla y_h \phi_i dx + \int_\Omega f(y_h, \theta)\phi_i dx = 0, \quad i = 1, \ldots, N.$$

To simplify presentation omit stabilization and often set $g(x_j) = 0$.

- In practice use quadrature to evaluate integrals:
$x_\ell \in \overline{\Omega}$, $\varpi_\ell \in \mathbb{R}$, $\ell = 1, \ldots, n_q$, quadrature nodes and weights.

$$F_h(y_h, \phi; \theta) = \sum_{\ell=1}^{n_q} \varpi_\ell f(y_h(x_\ell), \theta)\phi(x_\ell) \left(\approx \int_\Omega f(y_h(x), \theta)\phi(x) dx \right).$$

- Matrix form:

$$\mathbf{A}\mathbf{y} + \mathbf{F}(\mathbf{y}; \theta) = \mathbf{b}.$$

Basic Reduced Order Model

- Generate snapshots $y_{h,i}$, $i = 1, \ldots, n$ ($\mathbf{y}_i$, $i = 1, \ldots, n$)
- Extract orthonormal basis $v_{h,i}$, $i = 1, \ldots, n$ ($\mathbf{v}_i$, $i = 1, \ldots, n$) from snapshots. $n \ll N$.
- Approximate $\mathbf{y} = \bar{\mathbf{y}} + \mathbf{V}\widehat{\mathbf{y}}$. (To simplify notation set $\bar{\mathbf{y}} = \mathbf{0}$.)
- Reduced order model

$$\underbrace{\mathbf{V}^T\mathbf{A}\mathbf{V}}_{n\times n}\widehat{\mathbf{y}} + \mathbf{V}^T\mathbf{F}(\mathbf{V}\widehat{\mathbf{y}};\theta) = \mathbf{V}^T\mathbf{b}.$$

  where $\mathbf{V} = (\mathbf{v}_1, \ldots, \mathbf{v}_n) \in \mathbb{R}^{N\times n}$.
- Approximation of $\widehat{\mathbf{y}} \mapsto \mathbf{V}^T\mathbf{F}(\mathbf{V}\widehat{\mathbf{y}};\theta)$ with (on-line) computational complexity independent of N.
  EIM: Barrault, Maday, Nguyen, Patera (2004), Grepl et al. (2007).
  DEIM: Chaturantabut, Sorensen (2010).

DEIM

- Generate subspace $\mathbf{U} = [\mathbf{u}_1, \ldots, \mathbf{u}_m] \in \mathbb{R}^{N \times m}$ for nonlinear term. Want $\mathbf{F}(\mathbf{V}\widehat{\mathbf{y}}(\theta); \theta) \in R(\mathbf{U})$ approximately for all $\theta \in \Theta$.
- Compute approximation $\widehat{\mathbf{F}}(\mathbf{V}\widehat{\mathbf{y}}; \theta) = \mathbf{U}\mathbf{c}(\widehat{\mathbf{y}}; \theta)$ such that

$$\widehat{\mathbf{F}}_i(\mathbf{V}\widehat{\mathbf{y}}; \theta) = \mathbf{F}_i(\mathbf{V}\widehat{\mathbf{y}}; \theta) \text{ for components } i = p_1, \ldots, p_m.$$

  (Index selection next slide)
- Define $\mathbf{P} = [\mathbf{e}_{p_1}, \ldots, \mathbf{e}_{p_m}] \in \mathbb{R}^{N \times m}$; write interpolation condition as

$$\mathbf{P}^T \widehat{\mathbf{F}}(\mathbf{V}\widehat{\mathbf{y}}; \theta) = \mathbf{P}^T \mathbf{F}(\mathbf{V}\widehat{\mathbf{y}}; \theta).$$

- DEIM approximation of nonlinearity:

$$\widehat{\mathbf{F}}(\mathbf{V}\widehat{\mathbf{y}}; \theta) \stackrel{\text{def}}{=} \mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}\mathbf{P}^T \mathbf{F}(\mathbf{V}\widehat{\mathbf{y}}; \theta).$$

- DEIM reduced order model

$$\mathbf{V}^T\mathbf{A}\mathbf{V}\widehat{\mathbf{y}} + \underbrace{\mathbf{V}^T\mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}}_{n \times m}\mathbf{P}^T\mathbf{F}(\mathbf{V}\widehat{\mathbf{y}}; \theta) = \mathbf{V}^T\mathbf{b}.$$

Selection of DEIM points

Input: Linearly independent vectors $\mathbf{u}_1, \ldots, \mathbf{u}_m$.
Output: Indices $p_1, \ldots, p_m$.

1. $[\rho, p_1] = \max\{|\mathbf{u}_1|\}$
2. Set $\mathbf{U} = [\mathbf{u}_1]$, $\mathbf{P} = [\mathbf{e}_{p_1}]$, $\mathbf{p} = [p_1]$
3. For $i = 2, \ldots, m$ do
   - 3.1 Solve $(\mathbf{P}^T\mathbf{U})\mathbf{c} = \mathbf{P}^T\mathbf{u}_i$ for $\mathbf{c}$
   - 3.2 $\mathbf{r}_i = \mathbf{u}_i - \mathbf{U}\mathbf{c}$
   - 3.3 $[\rho, p_i] = \max\{|\mathbf{r}_i|\}$
   - 3.4 Update $\mathbf{U} = [\mathbf{U} \quad \mathbf{u}_i]$, $\mathbf{P} = [\mathbf{P} \quad \mathbf{e}_{p_i}]$, $\mathbf{p} = [\mathbf{p}^T \quad p_i]^T$

DEIM error estimate: If $\mathbf{U} \in \mathbb{R}^{N\times m}$ has ortho-normal columns, then

$$\|\mathbf{F} - \widehat{\mathbf{F}}\|_2 \leq \|(\mathbf{P}^T\mathbf{U})^{-1}\|_2 \|(\mathbf{I} - \mathbf{U}\mathbf{U}^T)\mathbf{F}\|_2 \,.$$

Why is DEIM efficient?

- DEIM approximation of nonlinearity:

$$\widehat{\mathbf{F}}(\mathbf{V}\widehat{\mathbf{y}};\theta) \stackrel{\text{def}}{=} \mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}\mathbf{P}^T\mathbf{F}(\mathbf{V}\widehat{\mathbf{y}};\theta).$$

- Need to evaluate m components $\mathbf{F}_{p_1}, \dots, \mathbf{F}_{p_m}$.
  If they depend on $k \approx n$ components of $\mathbf{V}\widehat{\mathbf{y}}$, then we only need to compute product of $k \times n$ submatrix of $\mathbf{V}$ times $\widehat{\mathbf{y}}$.

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- (Continuous nodal) FEM:

$$\mathbf{F}_i(\mathbf{y};\theta) = F_h(y_h, \phi_i;\theta) = \int_\Omega f\Big(\sum_{j=1}^N \mathbf{y}_j \phi_j(x), \theta\Big)\phi_i(x)dx$$

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- (Continuous nodal) FEM:

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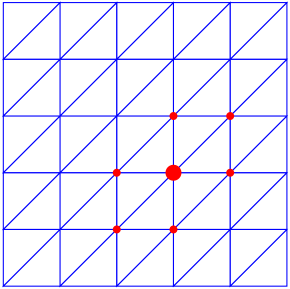
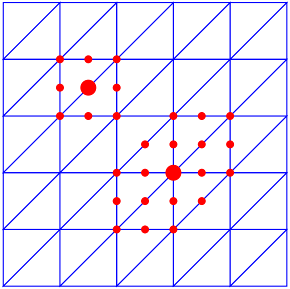
- P1  P2 

- Alternative:

$$\mathbf{F}_i(\mathbf{y};\theta) = \sum_{e=1}^{n_e} \underbrace{\int_{\Omega_e} f\Big(\sum_{j=1}^{N} \mathbf{y}_j \phi_j(x);\theta\Big)\phi_i(x)dx}_{\stackrel{\text{def}}{=} \mathbf{F}_i^e(\mathbf{y};\theta)}$$

  Assemble (add element information)

$$\mathbf{F}(\mathbf{y};\theta) = \mathbf{Q}\ \mathbf{F}^e(\mathbf{y};\theta)$$

  where $\mathbf{Q} \in \mathbb{R}^{N\times(n_e n_p)}$ (n_e # elements, n_p # DOF per element).
- Reduced order model applied to unassembled nonlinearity:
  - Basic model

$$\mathbf{V}^T\mathbf{A}(\mathbf{V}\widehat{\mathbf{y}}) + \mathbf{V}^T\mathbf{Q}\mathbf{F}^e(\mathbf{V}\widehat{\mathbf{y}};\theta) = \mathbf{V}^T\mathbf{b}.$$

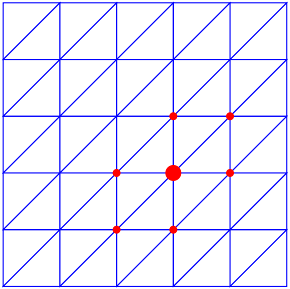
  - DEIM approximation of unassembled nonlinearity

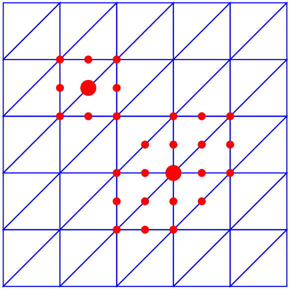
$$\widehat{\mathbf{F}}^e(\mathbf{y};\theta) = \mathbf{U}^e\big((\mathbf{P}^e)^T(\mathbf{U}^e)\big)^{-1}(\mathbf{P}^e)^T\mathbf{F}^e(\mathbf{y};\theta).$$

  - Final

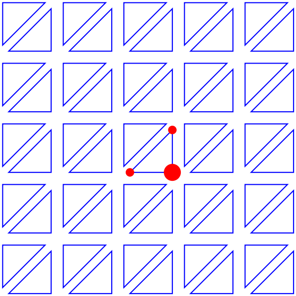
$$\mathbf{V}^T\mathbf{A}\mathbf{V}\widehat{\mathbf{y}} + \Big(\mathbf{V}^T\mathbf{Q}\mathbf{U}^e\big((\mathbf{P}^e)^T(\mathbf{U}^e)\big)^{-1}\Big)(\mathbf{P}^e)^T\mathbf{F}^e(\mathbf{V}\widehat{\mathbf{y}};\theta) = \mathbf{V}^T\mathbf{b}.$$

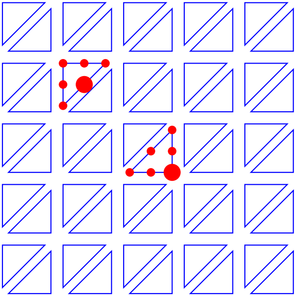
Connectivity Assembled





Connectivity Unassembled



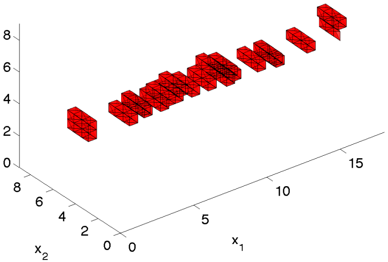


Apply to 3D Diffusion-Advection-Reaction PDE

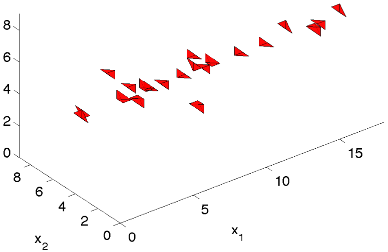
Piecewise linear FEM

Thetrahedra that need to be evaluated

assembled



unassembled



Polynomial degree		$p = 1$		$p = 2$	
Mesh number	1	2	3	1	2
# tetrahedra	6,144	49,152	165,888	6,144	49,152
# nodes N	1,296	9,248	30,000	9,248	69,696
# POD basis vectors n	19	18	19	18	19
# DEIM points m	21	21	22	21	22
# nodes adjacent DEIM pts.	183	271	320	445	559
# DEIM points m^e	21	21	22	21	22
# nodes adjacent DEIM pts.	67	80	88	193	220

EIM

- Works with nonlinearity $f(y, \theta)$
- Variational form

$$\begin{aligned}\mathbf{F}(\mathbf{y};\theta)_i =& F_h(y_h, \phi; \theta) \\ =& \sum_{\ell=1}^{n_q} \varpi_\ell f(y_h(x_\ell), \theta)\phi_i(x_\ell) \left(\approx \int_\Omega f(y_h(x), \theta)\phi_i(x) dx \right)\end{aligned}$$

- Define

$$\begin{aligned}\Phi &= \begin{pmatrix} \phi_1(\xi_1) & \dots & \phi_1(\xi_{n_q}) \\ \vdots & & \vdots \\ \phi_N(\xi_1) & \dots & \phi_N(\xi_{n_q}) \end{pmatrix} \in \mathbb{R}^{N \times n_q}, \\ \mathbf{W} &= \mathrm{diag}(\varpi_1, \dots, \varpi_{n_q}), \\ y_h &= (y_h(x_1), \dots, y_h(x_{n_q}))^T, \\ \mathbf{f}(y_h; \theta) &= (f(y_h(x_1), \theta), \dots, f(y_h(x_{n_q}), \theta))^T\end{aligned}$$

- FEM approx. at all quadrature points: $y_h = \Phi^T \mathbf{y}$.
  Matrix form of nonlinearity $\mathbf{F}(\mathbf{y}; \theta) = \Phi^T \mathbf{W} \mathbf{f}(y_h; \theta)$.

EIM

- Generate subspace $\widetilde{\mathbf{U}} = [\widetilde{\mathbf{u}}_1, \ldots, \widetilde{\mathbf{u}}_m] \in \mathbb{R}^{N \times n_q}$ for nonlinear term.
  Want $\mathbf{f}(y_h(\theta);\theta) \in R(\widetilde{\mathbf{U}})$ approximately for all $\theta \in \Theta$.
- Compute approximation $\widetilde{\mathbf{f}}(y_h(\theta);\theta) = \widetilde{\mathbf{U}}\mathbf{c}(y_h(\theta);\theta)$ such that

  $\widetilde{\mathbf{f}}(y_h(x_i);\theta) = \mathbf{f}(y_h(x_i);\theta)$ for components/quad. points $i = \widetilde{p}_1, \ldots, \widetilde{p}_m$.
- Define $\widetilde{\mathbf{P}} = [\mathbf{e}_{\widetilde{p}_1}, \ldots, \mathbf{e}_{\widetilde{p}_m}] \in \mathbb{R}^{N \times n_q}$; write interpolation condition as

$$\widetilde{\mathbf{P}}^T \widetilde{\mathbf{f}}(y_h;\theta) = \widetilde{\mathbf{P}}^T \mathbf{f}(y_h;\theta).$$

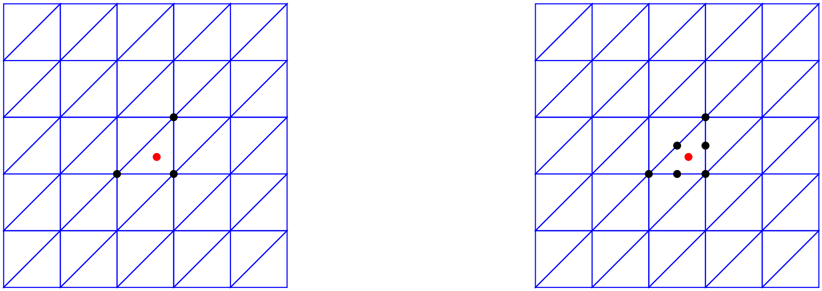
- EIM approximation of nonlinearity:

$$\widetilde{\mathbf{f}}(\widehat{y}_h;\theta) \stackrel{\text{def}}{=} \widetilde{\mathbf{U}}(\widetilde{\mathbf{P}}^T \widetilde{\mathbf{U}})^{-1} \widetilde{\mathbf{P}}^T \mathbf{f}(\mathbf{V}\widehat{y}_h;\theta).$$

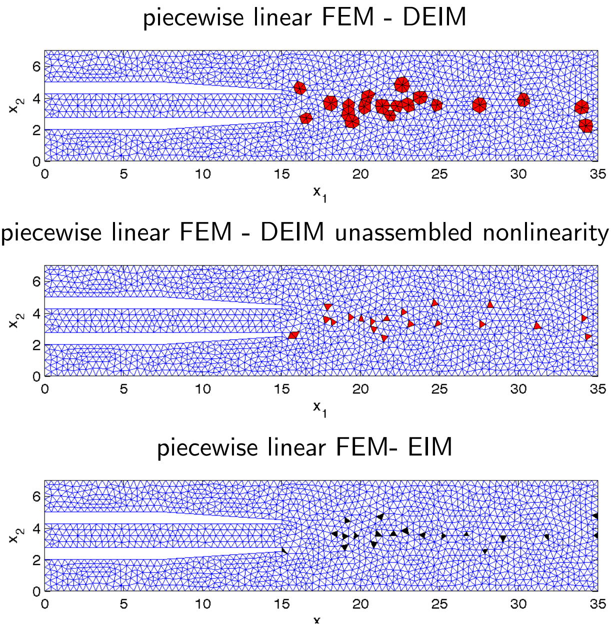
- FEM approx. at all quadrature points: $y_h = \Phi^T \mathbf{y}$, $\widehat{y}_h = \Phi^T \mathbf{V}\widehat{\mathbf{y}}$.
  At EIM quad. points $i = \widetilde{p}_1, \ldots, \widetilde{p}_m$: $\mathbf{Q}\Phi^T\mathbf{V}\widehat{\mathbf{y}}$.
- EIM reduced order model

$$\mathbf{V}^T\mathbf{A}\mathbf{V}\widehat{\mathbf{y}} + \underbrace{\mathbf{V}^T\Phi^T\mathbf{W}\widetilde{\mathbf{U}}(\widetilde{\mathbf{P}}^T\widetilde{\mathbf{U}})^{-1})^{-1}}_{n\times m} \widetilde{\mathbf{P}}^T\mathbf{f}(\Phi^T\mathbf{V}\widehat{\mathbf{y}};\theta) = \mathbf{V}^T\mathbf{b}.$$

Evaluations • for EIM (quadrature) point •



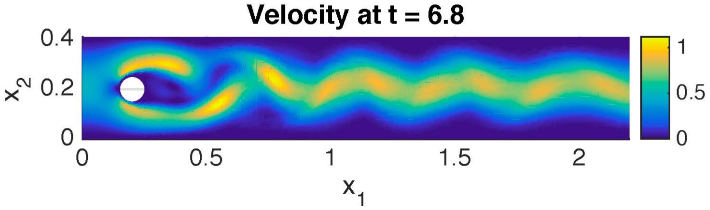
Apply to 2D Diffusion-Advection-Reaction PDE



Polynomial degree	$p = 1$			$p = 2$		
Mesh number	2	3	4	2	3	4
# triangles	3,213	12,976	53,120	3,213	12,976	53,120
# nodes N	1,768	6,813	27,215	6,751	26,604	107,552
# POD basis vectors n	16	17	17	17	17	17
# DEIM points m	19	20	20	20	20	20
# nodes adjacent DEIM pts.	130	160	162	168	177	180
# DEIM-u points m^e	20	20	20	20	20	20
# nodes adjacent DEIM-u pts.	56	60	60	114	120	120
# EIM points m	20	20	20	20	20	20

DEIM for Navier-Stokes

$$
\begin{aligned}
\frac{\partial}{\partial t} v(x,t) - \nu \Delta v(x,t) & \\
+(v(x,t)\cdot\nabla) v(x,t) + \nabla p(x,t) &= 0, && \text{in } \Omega \times [0,T], \\
\nabla \cdot v(x,t) &= 0, && \text{in } \Omega \times [0,T], \\
v(x,t) &= g(x,t), && \text{on } \Gamma_{in} \times [0,T], \\
v(x,t) &= 0, && \text{on } \Gamma_D \times [0,T], \\
(\nabla v(x,t) - p(x,t) I) n(x) &= 0, && \text{on } \Gamma_{out} \times [0,T].
\end{aligned}
$$



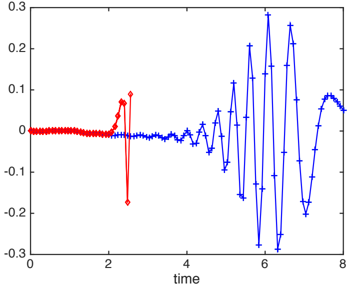
Set-up as in V. John (2004)

- Taylor-Hood P2-P1 finite elements leads to

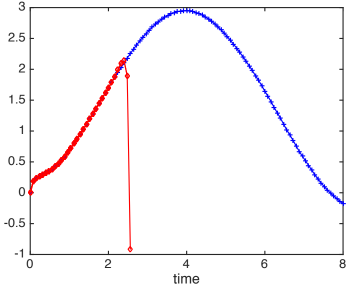
$$\begin{aligned}\mathbf{M}\frac{d}{dt}\mathbf{v}(t) + \mathbf{A}\mathbf{v}(t) + \mathbf{N}(\mathbf{v}(t))\mathbf{v}(t) + \mathbf{B}^T\mathbf{p}(t) &= \mathbf{f}(t),\\ \mathbf{B}\mathbf{v}(t) &= \mathbf{g}(t),\\ \mathbf{v}(0) &= \mathbf{0}.\end{aligned}$$

- Treat $\mathbf{v}(t) \mapsto \mathbf{N}(\mathbf{v}(t))\mathbf{v}(t)$ as general nonlinear term with DEIM

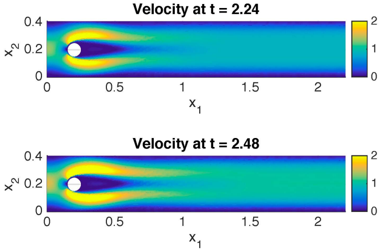
Lift (— full; — POD-DEIM)



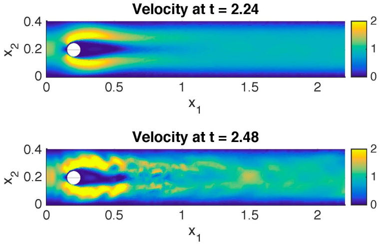
Drag (— full; — POD-DEIM)



full



POD-DEIM



- Have that

$$\int_\Omega (v(x)\cdot\nabla)w(x)\cdot w(x)dx = 0 \quad \text{for all } v \in [H^1(\Omega)]^2, w \in [H_0^1(\Omega)]^2$$

$$\text{with } \nabla\cdot v(x) = 0 \text{ in } \Omega.$$

- For Navier-Stokes with Dirichlet BCs everywhere,

$$\int_\Omega v^2(x,T)dx + \nu\int_0^T\int_\Omega \|\nabla v(x,t)\|^2 dxtdt \le \int_\Omega v^2(x,0)dx + \int_0^T\int_\Omega \|f(x,t)\|^2 dx$$

(Dropped several constants.)

- If discretely, $\mathbf{v}(t)^T\mathbf{N}(\mathbf{v}(t))\mathbf{v}(t) = 0$,

$$\|\mathbf{v}(T)\|^2 + \int_0^T \mathbf{v}(t)^T\mathbf{A}\mathbf{v}(t)dt \le \|\mathbf{v}(0)\|^2 + \int_0^T\int_0^T \|\mathbf{f}(t)\|^2 dt$$

- Have that

$$\int_\Omega (v(x)\cdot\nabla)w(x)\cdot w(x)dx = 0 \quad \text{for all } v\in[H^1(\Omega)]^2, w\in[H^1_0(\Omega)]^2$$
$$\text{with } \nabla\cdot v(x) = 0 \text{ in } \Omega.$$

- For Navier-Stokes with Dirichlet BCs everywhere,

$$\int_\Omega v^2(x,T)dx + \nu\int_0^T\int_\Omega \|\nabla v(x,t)\|^2 dxtdt \le \int_\Omega v^2(x,0)dx + \int_0^T\int_\Omega \|f(x,t)\|^2 dx$$

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- If discretely, $\mathbf{v}(t)^T\mathbf{N}(\mathbf{v}(t))\mathbf{v}(t) = 0$,

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- If $\mathbf{v}(t)^T\mathbf{N}(\mathbf{v}(t))\mathbf{v}(t) = 0$ for all snapshots, then $(\mathbf{V}\widehat{\mathbf{v}}(t))^T\mathbf{N}(\mathbf{V}\widehat{\mathbf{v}}(t))\mathbf{V}\widehat{\mathbf{v}}(t) = 0$ for POD.

- Have that
$$\int_\Omega (v(x)\cdot\nabla)w(x)\cdot w(x)dx = 0 \quad \text{for all } v\in[H^1(\Omega)]^2, w\in[H_0^1(\Omega)]^2$$
$$\text{with } \nabla\cdot v(x) = 0 \text{ in } \Omega.$$
- For Navier-Stokes with Dirichlet BCs everywhere,
$$\int_\Omega v^2(x,T)dx + \nu\int_0^T\int_\Omega \|\nabla v(x,t)\|^2 dxtdt \le \int_\Omega v^2(x,0)dx + \int_0^T\int_\Omega \|f(x,t)\|^2 dx$$
(Dropped several constants.)
- If discretely, $\mathbf{v}(t)^T\mathbf{N}(\mathbf{v}(t))\mathbf{v}(t) = 0$,
$$\|\mathbf{v}(T)\|^2 + \int_0^T \mathbf{v}(t)^T\mathbf{A}\mathbf{v}(t)dt \le \|\mathbf{v}(0)\|^2 + \int_0^T\int_0^T \|\mathbf{f}(t)\|^2 dt$$
- If $\mathbf{v}(t)^T\mathbf{N}(\mathbf{v}(t))\mathbf{v}(t) = 0$ for all snapshots, then $(\mathbf{V}\widehat{\mathbf{v}}(t))^T\mathbf{N}(\mathbf{V}\widehat{\mathbf{v}}(t))\mathbf{V}\widehat{\mathbf{v}}(t) = 0$ for POD.
- DEIM approximation of nonlinearity:
$$\mathbf{N}(\mathbf{v}(t))\mathbf{v}(t) \approx \mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}\mathbf{P}^T\Big(\mathbf{N}(\mathbf{V}\widehat{\mathbf{v}}(t))\mathbf{V}\widehat{\mathbf{v}}(t)\Big).$$
In general
$$\widehat{\mathbf{v}}(t)\mathbf{V}^T\mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}\mathbf{P}^T\Big(\mathbf{N}(\mathbf{V}\widehat{\mathbf{v}}(t))\mathbf{V}\widehat{\mathbf{v}}(t)\Big) \ne 0.$$

Outline

Error Estimate

- Original problem $\mathbf{G}(\mathbf{y},\theta) = \mathbf{A}\mathbf{y} + \mathbf{F}(\mathbf{y},\theta) - \mathbf{b} = \mathbf{0}$.
  Solution $\mathbf{y}^*$.
- POD-DEIM reduced order model

$$
\begin{aligned}
&\mathbf{V}_n^T \mathbf{G}(\overline{\mathbf{y}} + \mathbf{V}_n \widehat{\mathbf{y}}, \theta) \\
=&\mathbf{V}_n^T \mathbf{A} \mathbf{V}_n \widehat{\mathbf{y}} + \mathbf{V}_n^T \mathbf{U}_m (\mathbf{P}^T \mathbf{U}_m)^{-1} \mathbf{P}^T \mathbf{F}(\overline{\mathbf{y}} + \mathbf{V}_n \widehat{\mathbf{y}}, \theta) \\
&+ \mathbf{V}_n^T \mathbf{A} \overline{\mathbf{y}} + \mathbf{V}_n^T \mathbf{b} = \mathbf{0}.
\end{aligned}
$$

  Solution $\widehat{\mathbf{y}}^*$.
  Will drop mean $\overline{\mathbf{y}}$ to simplify notation.
- Want estimate $\mathbf{y}^* - \mathbf{V}_n \widehat{\mathbf{y}}^*$; select number of bases $\mathbf{V}_n, \mathbf{U}_m$.

Newton's Method

- Newton's method for the original problem

$$\begin{aligned} D_y \mathbf{G}(\mathbf{y}^k, \theta)\delta \mathbf{y}^k &= -\mathbf{G}(\mathbf{y}^k, \theta), \\ \mathbf{y}^{k+1} &= \mathbf{y}^k + \delta \mathbf{y}^k. \end{aligned}$$

- Newton's method for the POD-DEIM reduced order model

$$\begin{aligned} D_y \mathbf{V}_n^T \mathbf{F}(\mathbf{V}_n \widehat{\mathbf{y}}^k, \theta)\mathbf{V}_n \delta \widehat{\mathbf{y}} &= -\mathbf{V}_n^T \mathbf{F}(\mathbf{V}_n \widehat{\mathbf{y}}^k, \theta), \\ \widehat{\mathbf{y}}^{k+1} &= \widehat{\mathbf{y}}^k + \delta \widehat{\mathbf{y}}^k. \end{aligned}$$

Newton-Kantorowich type estimates

- $\mathbf{G}(\mathbf{y}, \theta)$ cont. diff'bel ; $D_y \mathbf{G}(\mathbf{y}, \theta)$ be invertible for all $\mathbf{y}$, $\theta \in \Theta$.
- Affine covariance Lipschitz condition

$$\left\| D_y \mathbf{G}(\mathbf{y}, \theta)^{-1} (D_y \mathbf{G}(\mathbf{y}, \theta) - D_y \mathbf{G}(\mathbf{v}, \theta))(\mathbf{y} - \mathbf{v}) \right\| \leq \omega \|\mathbf{y} - \mathbf{v}\|^2 \quad \forall \mathbf{y}, \mathbf{v}.$$

- $h_0 = \omega \|\delta \mathbf{y}^0\| < 2.$

Newton's method converges to $\mathbf{y}^*$ with quadratic convergence rate

$$\|\mathbf{y}^{k+1} - \mathbf{y}^k\| \leq \frac{\omega}{2} \|\mathbf{y}^k - \mathbf{y}^{k-1}\|^2$$

and

$$\left\| \mathbf{y}^* - \mathbf{y}^0 \right\| \leq \widehat{r}_0 \stackrel{\text{def}}{=} \frac{\|\delta \mathbf{y}^0\|}{1 - \frac{1}{2} h_0}.$$

Can estimate (heuristics)

$$h_0 \approx 2\Theta_0 \quad \text{with } \Theta_0 = \|\delta \mathbf{y}^1\|_2 / \|\delta \mathbf{y}^0\|_2.$$

Error Estimates

- Apply previous theorem to full problem with star value $\mathbf{y}^0 = \mathbf{V}_n \widehat{\mathbf{y}}^*$:

$$\|\mathbf{y}^* - \mathbf{V}_n \widehat{\mathbf{y}}^*\| \le r_0 \stackrel{\text{def}}{=} \frac{\|\delta \mathbf{y}^0\|}{1 - \frac{1}{2} h_0}.$$

  Can estimate (heuristics)

$$h_0 \approx 2\Theta_0 \quad \text{with } \Theta_0 = \|\delta \mathbf{y}^1\|_2 / \|\delta \mathbf{y}^0\|_2.$$

- Apply previous theorem to reduced order problem with star value $\widehat{\mathbf{y}}^0 = \mathbf{V}_n^T \mathbf{y}^*$:

$$\left\|\widehat{\mathbf{y}}^* - \mathbf{V}_n^T \mathbf{y}^*\right\| \le \widehat{r}_0 \stackrel{\text{def}}{=} \frac{\|\delta \widehat{\mathbf{y}}^0\|}{1 - \frac{1}{2} \widehat{h}_0}.$$

  Can estimate (heuristics)

$$\widehat{h}_0 \approx 2\widehat{\Theta}_0 \quad \text{with } \widehat{\Theta}_0 = \|\delta \widehat{\mathbf{y}}^1\|_2 / \|\delta \widehat{\mathbf{y}}^0\|_2.$$

Heuristic Algorithm

INPUT: Newton tolerance: τ_{new}, max. Newton iterations: k_{max},
tolerance: τ_{est},
initial size of basis: n, max. size basis: $n_{max} > n$,
initial Newton iterate: $\widehat{\mathbf{y}}^0$
OUTPUT: r_0, $\mathbf{V}_n$

while $n \leq n_{max}$

- Generate reduced order model $\mathbf{V}_n$, $\mathbf{U}_m$
- Apply Newton's method to compute $\widehat{\mathbf{y}}^*$.
- Estimate error (full estimator)
  - Set $\mathbf{y}^0 = \overline{\mathbf{y}} + \mathbf{V}_n \widehat{\mathbf{y}}^*$
  - Compte $\Theta_0 = \frac{\|\delta \mathbf{y}^1\|_2}{\|\delta \mathbf{y}^0\|_2}$, $r_0 = \frac{\|\delta \mathbf{y}^0\|_2}{1-\Theta_0}$
  - **If** $r_0 \leq \tau_{est}$, **STOP (outer loop)**
  - **else if** $n+1 > n_{n_{max}}$, **update** basis $\mathbf{V}_{n_{max}}$.
  - **else** set $n = n+1$ goto 'while' loop
  - Compute the new iterate $\mathbf{y}^2 = \mathbf{y}^1 + \delta \mathbf{y}^1$.
  - $\widehat{\mathbf{y}}^0 = \mathbf{V}_n^T \mathbf{y}^2$.
- Estimate error (reduced estimator)
  Use reduced order problem with $\mathbf{V}_{n_{max}}$ instead of full order problem.

end

Application to 3D Reaction diffusion

Grid 1		Grid 2		Grid 3	
n	m	n	m	n	m
6	8	6	8	6	8
9	12	9	12	9	13
13	15	13	15	13	17
17	20	17	20	18	21
-	-	-	-	21	24

basis vectors n and # of DEIM points m for three different grids.

Grid 1		Grid 2		Grid 3	
estimate	actual (full)	estimate	actual (full)	estimate	actual (full)
3.53×10^{-2}	3.46×10^{-2}	1.54×10^{-2}	1.54×10^{-2}	3.12×10^{-1}	3.02×10^{-1}
2.22×10^{-3}	2.22×10^{-3}	5.23×10^{-3}	5.23×10^{-3}	1.66×10^{-2}	1.66×10^{-2}
5.27×10^{-4}	5.27×10^{-4}	2.29×10^{-3}	2.28×10^{-3}	8.95×10^{-3}	8.94×10^{-3}
-	-	2.77×10^{-4}	2.77×10^{-4}	1.72×10^{-3}	1.71×10^{-3}
-	-	-	-	9.47×10^{-4}	9.47×10^{-4}

Error estimator for three different grids using $\tau_{est} = 5 \times 10^{-4}$.

Conclusions:

- Comparison of DEIM and EIM for FEM computations
- Capture properties of full order problem in reduced order model.
- Newton-based error estimates